Pergamon

Computers Math. Applic. Vol. 36, No. 5, pp. 23–34, 1998

Printed in Great Britain
0898-1221/98 $19.00 + 0.00

PII: S0898-1221(98)00147-3

Improvement of Accuracy in Numerical Methods for Inverting Laplace Transforms Based on the Post-Widder Formula

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(Received June 1995; revised and accepted May 1998)

Abstract—The paper proposes a new computational version for numerical inversion of Laplace transforms at a point and on an interval, based on the Post-Widder formula. In this version the original sequence of Post-Widder approximants is calculated using operations on series and the approximate value of the sought function is constructed as a limit of this sequence using polynomial and rational extrapolation to the limit. Some procedures are proposed for improvement of accuracy in the problem of inversion at equidistant points of an interval without computing additional approximants. An extension of the method to the two-dimensional case is discussed. The one-dimensional version is illustrated with some probabilistic examples involving both explicit and implicit functions. The accuracy achieved in these examples with using the standard double precision arithmetic, evaluated in terms of relative errors, is about 10^{-10}–10^{-14} even in case of out-of-scale parameters. Computational aspects are discussed in comparison with previously known realizations of the Post-Widder method. © 1998 Elsevier Science Ltd. All rights reserved.

Keywords—Laplace transform, Numerical inversion of transforms, Enhancement procedure, Extrapolation to the limit, Post-Widder method, Gaver-Stehfest method, The Padé approximation.

1. INTRODUCTION

The Post-Widder method, or perhaps more precisely, family of methods for inverting Laplace transforms is based on approximation of the (unknown) original function $f(\cdot)$ defined on $[0,\infty)$ by approximants $f_k(\cdot)$, $k = 1, 2, \dots$, of the form

$$f_k(t) = s\frac{(-s)^{k-1}\widehat{f}^{(k-1)}(s)}{(k-1)!}\Bigg|_{s=k/t}, \qquad t > 0, \tag{1}$$

where $\widehat{f}$ is the (known) Laplace transform of the f and $\widehat{f}^{(i)}$ its i^{th} derivative, $i \ge 1$ ($\widehat{f}^{(0)} = \widehat{f}$). It is known that under some conditions $f_k(t) \to f(t)$ as $k \to \infty$; [1, Chapter VII, equation (6.6)].

Until relatively recent time this approach had questionable reputation. First, its "obvious disadvantage is the need to differentiate $\widehat{f}$ repeatedly" [2] and, second, the convergence of f_k to f is rather slow.

In the modern approach, the first of these problems is circumvented by using stable methods for direct computation or evaluation of approximants (1) without differentiating numerically. For

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example, Jagerman [3] among other things has proposed computing $f_k(t)$ by means of contour integrals in the complex plane. In practice this idea may be realized as trigonometric interpolation. In this paper, we consider an alternative approach.

The second problem is solved by applying so-called enhancement procedures speeding up the convergence. Gaver [4] was the first to invoke Richardson's technique of "extrapolation to the limit" widely used in different areas of numerical analysis [5] for the inversion problem. Other enhancement procedures for the Laplace transform inversion problem have been proposed by Stehfest [6], Jagerman [3], Abate and Whitt [7]. In the cited works the approximation to the sought value is constructed as a linear combination of f_k's.

In this paper, it is shown that the approximation by linear combinations in the framework of Richardson's technique is equivalent to the polynomial extrapolation and that the extrapolation by rational functions (the Padé approximation) is more efficient. Further improvement of accuracy is achieved by using operations on series for computing the Post-Widder approximants. This technique was previously used in the context of the Laguerre series method [8]. For the Post-Widder method the series technique allows one to compute precise (up to roundoff errors) values of approximants. The ease of adaptation of this approach to the inversion problem on intervals and in multidimensional areas is its other important advantage.

We focus on guiding ideas rather than mathematical aspects. Formulas are used only as motivations and given without derivations which are either well known (and then may be found, e.g., in [3,7,9]) or trivial.

In Section 2, the problem of obtaining original approximants (1) is considered. In Section 3, for the problem of inversion at a single point, several enhancement techniques are discussed based on extrapolation to the limit. Section 4 considers some features of the inversion problem on a finite interval. In Section 5, it is shown that most of techniques presented in foregoing sections may work in higher dimensions. In Section 6, our recommendations are illustrated with some numerical examples. All computations have been performed on the standard double precision arithmetic.

2. PROCEDURES FOR CALCULATING ORIGINAL APPROXIMANTS

Currently, there are two principal approaches known to the authors to numerically compute the approximants $f_k(t)$ defined by (1), each may include different modifications and implementations:

(FD) via Finite Differences;

(TI) via Trigonometric Interpolation;

(CS) via "Calculus of Series".

Method (FD) suffers from roundoff errors more than two other ones and for this reason is now out of practice. Method (TI) proposed by Jagerman [3,9] is based on the observation that, as follows from (1), the expression $s\widehat{f}(s(1-z))$ being considered as a function of z is the generating function of the sequence of approximants (up to a minor change of arguments), more exactly [3,7,9]

$$s\widehat{f}(s(1-z)) = \sum_{n\geq 1} f_n\left(\frac{n}{s}\right) z^{n-1}. \tag{2}$$

From here coefficients may be found by using contour integrals and different numerical techniques for computing them or by trigonometric interpolation. For example, taking q points for interpolation and denoting $h = 2\pi/q$ one obtains

$$\frac{s}{qr^{k-1}} \sum_{n=1}^{q} \widehat{f}\left(s\left(1 - re^{-inh}\right)\right) e^{-i(k-1)nh} = f_k\left(\frac{k}{s}\right) + \sum_{m\geq 1} f_{k+mq}\left(\frac{k+mq}{s}\right) r^{mq}. \tag{3}$$

Jagerman [9] recommends (3) for computing an approximate value of the approximant $f_k(t)$ (in which case s must be set to k/t) since remaining members in (3) can be reduced by a suitable choice of q and r. Theoretically, the right side of (3) becomes the closer to $f_k(t)$ the lesser r, however, roundoff errors hinder to make the radius r arbitrary small. In practice an adequate choice of r is a rather unclear question inasmuch properties of the function f and the value of t also have influence. When using arbitrary precision arithmetic Abate and Whitt [7] give a simple rule: to reduce the reminder in (3) to $10^{-\nu}$ it is necessary to perform computations with up to $3\nu/2$ decimal places accuracy. When using standard double precision arithmetic to improve accuracy, one can use extrapolation to the limit, for (3) has just that structure with respect to r which is required for applying this technique (see (7) in the next section). For example, the corresponding approximate formula for $f_k(t)$ using two radii r_1 and r_2 has the error estimate $O(r_1^q r_2^q)$ and is as follows:

$$f_k(t) \approx \frac{T_k(r_1)r_2^q - T_k(r_2)r_1^q}{r_2^q - r_1^q},$$

where $T_k(r)$ denotes the left hand side of (2) computed for $s = k/t$ and radius r.

Method (CS) also is based on (2). When $\widehat{f}$ has a simple analytic expression the expansion (2) can be obtained by hand. When $\widehat{f}$ is complex enough it should be broken up into a number of constituents each of which is explicitly expanded in the series. Then the final expansion (2) is constructed from the constituents using algebraic operations on series. In this case the series are transformed automatically by the computer according to well-known formulas; see, e.g., [10, 4.10–2] or [8]. The same approach also applies to implicit functions $\widehat{f}$; see [11].

For example, to evaluate a so called renewal function discussed in [3], $M(t)$, with the Laplace transform $\widehat{M}(s) = \nu(\mu + s)/(\nu s^2 + s^3)$, one needs to compute the approximants $m_k(\cdot)$ from the expansion (2) for $s_0\widehat{M}(s_0(1-z))$. Equation (2) takes the form

$$s_0\widehat{M}(s_0(1-z)) = \frac{\nu}{s_0}\frac{A(z)}{B(z)},$$

where

$$A(z) = a_0 + a_1 z, \qquad a_0 = \mu + s_0, \qquad a_1 = -s_0,$$
$$B(z) = b_0 + b_1 z + b_2 z^2, \qquad b_0 = \nu s_0 + s_0^2, \qquad b_1 = -(\nu s_0 + 2s_0^2), \qquad b_2 = s_0^2.$$

Then $C(z) := A(z)/B(z) = c_0 + c_1 z + \cdots$, where $c_0 = a_0/b_0$, and the remaining coefficients c_k are obtained by synthetic division of polynomials $A(z)$ by $B(z)$ [10]:

$$c_k = \frac{\left(a_k - \sum_{i=1}^k b_i c_{k-i}\right)}{b_0}, \qquad k \geq 1. \tag{4}$$

Whence, to evaluate the approximant $m_k(\cdot)$ at a point t we perform the above computations at $s_0 = k/t$, so $m_k(t) = \nu c_k/s_0$.

In the context of the Laplace transforms inversion problem the idea to use (CS) was recommended by Lanczos [12] in connection with the Laguerre series method and was systematically used and implemented as a computer program (LAGRA) by Piessens and Branders [8]. Keilson and Nunn [13] also recommended this technique. In the context of the Post-Widder method, this approach appeared in [14], where the basic set of operations (summation, multiplication, division) was enlarged to include in this "calculus" basic elementary functions (exp, sin, etc.) and more complex operations for working with implicit functions.

Method (CS) has the following evident advantages: unlike (TI), where accuracy is limited by the discretization error, it gives exact values of approximants (1); when computing $f_k(t)$ from (2) the computation is organized as a recursive procedure so that it gives as a side product all numbers $f_k(tj/k)$ for $1 \leq j \leq k$ which can be used to invert the Laplace transform on the whole interval $(0, t]$ without additional computational work (see Section 4). A serious disadvantage is that the operation of synthetic division frequently arising in computations may lead to unstable computational processes. Usually the instability can be overcome at the cost of significant complication of the algorithm in which case the method loses its attractive simplicity. In such cases method (TI) can be applied. On the other hand, method (CS) works where a straightforward application of (TI) fails to work as is the case for mixtures of out-of-scale distributions in an example constructed by Abate and Whitt [7] to reveal limitations of the Fourier-series method. Numerical results obtained with the Post-Widder method based on the (CS) techniques for this example are contained in Table 4. The results shown in Tables 2 and 3 are also obtained using (CS).

3. ENHANCEMENT PROCEDURES FOR THE PROBLEM OF INVERSION AT A SINGLE POINT

Enhancement procedures are based on more or less explicit representations of the discrepancy between $f_k(t)$ and $f(t)$.

For functions f infinitely differentiable at point t the following representation is the case [7,9]

$$f_k(t) = f(t) + \sum_{n\geq 1} \frac{a_n(t)}{k^n} \tag{5}$$

with coefficients of the form

$$a_n(t) = \sum_{m=1}^{n} f^{(n+m)}(t) t^{m+n} \frac{d(m+n,m)}{(m+n)!}. \tag{6}$$

where $d(n,m)$ are the adjoint Stirling numbers of the first kind (see [15, Section 4, Chapter 4]). To give an idea of the magnitude of the numbers in (6) note that $e_n(m) := d(n+m,m)/(n+m)!$ are positive and their sums $\sum_{m=1}^{n} e_n(m)$ decrease from $1/2$ to e^{-1} as $n \to \infty$. For applying the techniques under consideration the explicit form of the coefficients is immaterial and only the fact of their independence of k is important.

Remark that if the function f is not infinitely differentiable, then (5) is not the case and the situation is rather uncertain. When f has, say K, continuous derivatives, an examination in the spirit of Gaver's analysis [4] leads to an expression very similar to (5), but with truncated series and a reminder, and with coefficients no more satisfying (6). They may even depend on k starting with some number. In this situation, the technique presented below may as well as may not be efficient. In order to evade a discussion on this subject and to simplify further considerations, we shall simply assume (5).

As is observed [6,7], better approximations to $f(t)$ are attainable by taking linear combinations of $f_k(t)$ for different k because by a suitable choice of their coefficients it is possible to cancel out first few members on the right side of (5). Stehfest [6] found the optimal set of coefficients, see (14) below, in the sense that it eliminates on the right in (5) $n-1$ members using approximants of order not greater than n [7], whereas other choices require approximants of higher order. However, for computational reasons, these coefficients are limited in use. It is pointed out in [7, p. 60] that in order to have final results with accuracy of seven or eight significant figures for 16 approximants it is necessary to retain 28 figures in intermediate computations.

This difficulty is overcome by recasting the problem into an interpolation setting adopted in the theory of extrapolation to the limit. There is a huge literature on this subject [5, pp. 16–19]. As applied to the Laplace transform inversion this idea was proposed by Gaver [4].

The substitution $h = 1/k$ in (5) gives this formula a more "traditional" appearance for this theory [5,16,17]

$$T(h) := f_k(t) = f(t) + \sum_{n\geq 1} a_n(t) h^n. \tag{7}$$

The objective is to evaluate $T(0)$ (in our case $T(0) = f(t)$) in the situation when values of $T(h_i)$ ($T(h_i) = f_{k_i}(t)$) are available for computation at different points $h_i = 1/k_i$ and the function $T(\cdot)$ itself is unknown.

In the framework of this approach the above idea of eliminating as more as possible members on the right side of (7) by linear combinations of $T(h_i)$ is equivalent to interpolation by polynomials. Thus a natural generalizing step is to admit other forms of interpolating functions.

We first recall the reader how linear combinations of approximants are constructed furnishing a better approximation to $T(0)$ than $T(h_i)$, $i = 1, 2, \dots$, and show in parallel that this approach is equivalent to the polynomial interpolation. Rewrite (7) as

$$T(h) = T_n(h) + R_n(h) \tag{8}$$

where

$$T_n(h) = T(0) + \sum_{m=1}^{n-1} a_m(t)h^m, \qquad R_n(h) = \sum_{m\geq n} a_m(t)h^m. \tag{9}$$

If for given n and $h_1, \dots, h_n$, the numbers $c_1, \dots, c_n$ are chosen so as to satisfy the condition

$$\sum_{i=1}^{n} c_i T_n(h_i) = T_n(0) \;\; (= T(0) = f(t)), \tag{10}$$

then from here and (8) one obtains

$$\sum_{i=1}^{n} c_i T(h_i) = \sum_{i=1}^{n} c_i f_{k_i}(t) = f(t) + \sum_{i=1}^{n} c_i R_n(h_i). \tag{11}$$

From writing $T_n(h)$ as the Lagrange polynomial for itself

$$T_n(h) = \sum_{i=1}^{n} \left(\prod_{j\neq i} \frac{h - h_j}{h_i - h_j} \right) T_n(h_i)$$

the explicit form of the unknown coefficients $c_1, \dots, c_n$ immediately follows by taking here $h = 0$ and comparing with (10)

$$c_i = \prod_{j\neq i} \frac{-h_j}{h_i - h_j} = \prod_{j\neq i} \frac{-k_i}{k_j - k_i} = \frac{(-k_i)^{n-1}}{\prod_{j\neq i}(k_j - k_i)}. \tag{12}$$

It is also clear now that the left-hand side of (11) with these coefficients c_i coincides with the value taken at zero by the Lagrange polynomial of degree $n-1$ constructed for $T(h)$. This approach leads to the error estimate given by the second member on the right-hand side in (11), which after some algebra transforms into:

$$\sum_{i=1}^{n} c_i R_n(h_i) = (-1)^{n-1} \prod_{i=1}^{n} h_i \sum_{m\geq n} a_m(t) h^{m-1}[h_1; h_2, \dots, h_n] \tag{13}$$

(here $h^{m-1}[h_1; h_2; \dots; h_n]$, $n \geq 2$ denotes the n^{th} divided difference of the power function h^{m-1} computed at points $h_1, \dots, h_n$).

There are two well-known variants to choose the sequence $k_1, \dots, k_n$: $k_i = i$ (Stehfest) and $k_i = 2^{i-1}$ (Romberg). Respectively,

$$c_i^S = (-1)^{n-i} \binom{n}{i} \frac{i^n}{n!}, \quad c_i^R = \frac{(-1)^{n-i} 2^{i(i-1)/2}}{\prod_{j=1}^{i-1}(2^j - 1) \prod_{j=1}^{n-i}(2^j - 1)}, \qquad 1 \leq i \leq n. \tag{14}$$

A rapid growth of the coefficients c_i^S (which may be seen using the Stirling formula) leads to aforementioned computational difficulties. Such a problem does not arise for c_i^R but in this case approximants of high order are required (e.g., for $n = 11$ one needs to evaluate $f_{1024}(t)$), and thus the primary source of errors lies just at this point. However, if there is a stable procedure for obtaining the approximants, the coefficients c_i^R appear to be more preferable than c_i^S as providing a better accuracy for the same n (see Table 1). Note that for Romberg's nodes h_i a repeated application of well-known Aitken's Δ^2-process leads to the same final result.

The multiple $B_n = \prod_{i=1}^n h_i$ in (13), while independent of the function in question, characterizes to some extent the choice of $\{k_i\}$. In Table 1 the values of B_n are shown for Stehfest, Romberg, and two another sequences (cf. with Table 2 where the real accuracy is shown). The first sequence, "backward Stephest", is optimal when we wish to minimize the absolute value of B_n for some fixed n as a function of $h_1, \dots, h_n$ subject to the maximal order of approximant does not exceed some K (in Table 1 $K = 101$). From computational point of view so obtained coefficients have the same shortcoming as Stehfest's ones. The second sequence approaches in the sense of accuracy the backward Stehfest case being at the same time more stable. In any case, experience suggests that with using double precision arithmetic there is no point in increasing n more than 10–12.

Table 1. Absolute value of the multiple $B_n = \prod_{i=1}^n h_i$ in the reminder for the polynomial extrapolation.

Sequence k_i	$n = 2$	$n = 4$	$n = 6$	$n = 8$	$n = 10$
Stehfest	0.5	4e − 2	1e − 3	3e − 5	3e − 7
Romberg	0.5	2e − 2	3e − 5	4e − 9	3e − 12
$k_i = 101 - i (i = 1, n)$	1e − 2	1e − 6	1e − 10	1e − 14	1e − 18
$k_i = 10i \ (i = 1, n)$	5e − 3	4e − 6	1e − 9	3e − 13	3e − 17

Table 2. Absolute values of relative and absolute errors (at the top respectively bottom in each cell) of inverted Laplace transforms using rational extrapolation and $k_i = 10i$, $i < 16$. Here $M(t) = (20/17)t + (1 - \exp(-1.7t))21/289$ is the renewal function with Laplace transform $\widehat{M}(s) = (20+13s)/(s^2(17+10s))$; $p(t)$ is the original of $\pi(s)$ determined from (21) $\lambda = 0.99$, $\beta(s) = 1/(1+s)$.

$f(t) =$	$\exp(-t)$	$J_0(t)$	$M(t)$	$p(t)$
$t = 0.1$	4e − 15	2e − 13	3e − 13	4e − 14
	4e − 15	2e − 13	4e − 14	6e − 14
$t = 1.0$	2e − 14	4e − 13	5e − 13	3e − 14
	7e − 15	5e − 13	7e − 13	8e − 15
$t = 5.0$	4e − 12	1e − 11	9e − 13	9e − 12
	2e − 14	2e − 12	5e − 12	2e − 13
$t = 10$	2e − 11	4e − 10	4e − 13	2e − 12
	7e − 16	9e − 11	5e − 11	2e − 14
$t = 20$	4e − 9	1e − 7	4e − 14	3e − 13
	7e − 18	2e − 8	5e − 12	1e − 16
$t = 40$	4e − 3	1e − 2	1e − 14	6e − 14
	2e − 20	6e − 5	9e − 13	7e − 17

Intuitively, the source of errors is that polynomials constructed as interpolating ones are used for extrapolation. The higher the degree of an interpolating polynomial the faster this polynomial loses its oscillatory properties outside the region of interpolation and with it approximating abilities and goes to an infinity. From this point of view the Stehfest sequence is the worst possible since its nodes h_i are widely spaced from the extrapolated point $h = 0$.

The choice of rational functions to approximate $T(\cdot)$ (the Padé approximation [20]) by means of interpolation enable one to overcome the indicated drawbacks of polynomial extrapolation. For the purposes of extrapolation to the limit the Padé approximation was used by different authors (see the survey by Joyce [5]) for improving accuracy in problems of numerical integration, differentiation and solving differential equations.

We outline here a procedure very similar to that due to Bulirsch and Stoer [21] for finding the value of the approximating rational function at zero. Other algorithms and more general settings can be found in [20]. Let $T_k^i(h)$ denote the rational function with degrees of numerator and denominator $[k/2]$ and $k - [k/2]$, respectively, constructed by interpolating at points $(h_i, T(h_i)), \ldots, (h_{i+k}, T(h_{i+k}))$, and T_k^i its value at zero. These quantities will appear in the process of computations as elements of Aitken-Neville's table [5]:

$$T_{-1}^i = 0, \quad T_0^i = T(h_i) = f_i(t), \qquad 1 \le i \le n,$$

$$T_m^i = T_{m-1}^{i+1} + \frac{T_{m-1}^{i+1} - T_{m-1}^i}{h_i/(h_{i+m})(T_{m-1}^i - T_{m-2}^{i+1})/(T_{m-1}^{i+1} - T_{m-2}^{i+1} - 1)},$$

$$1 \le m \le n-1, \qquad 1 \le i \le n-m.$$

The result of this procedure is the value $T_{n-1}^1 \approx T(0)$. Theoretically, this scheme converges as $n \to \infty$ if and only if $\sup_i (h_i/h_{i+1}) < 1$; see [22]. It is interesting to note that among the above sequences only Romberg's one has this property.

Usually the computation terminates before reaching the last column of the table when computational errors become prevalent. The total error may be tracked by evaluating upper and lower bounds for the sought value [5,21]. These bounds, in turn, may be derived from the explicit expression for the method error estimate which in the general case of the Padé approximation can be found in [20]. For the case when (7) holds this estimate at point 0 takes the form [17]

$$T_k^i - T(0) = h_i, \ldots, h_{i+k} \left(e_{k+1,0} + O\left(\max_j h_j \right) \right), \tag{15}$$

This expression shows that if $e_{k+1,0} \neq 0$, and h_j tends to zero, then for fixed k the extrapolating value T_k^i tends monotonically to the exact value $T(0)$ and thus may serve as one of the bounds. Violation of the monotonicity indicates either a critical accumulation of computational errors or that $h_i, \ldots, h_{i+k}$ are not sufficiently small and so the elder terms in the expansion (15) affect the behavior.

In order to control the error as the exact value is approached, Bulirsch and Stoer [21] constructed a bound U_k^i on $T(0)$ opposite to T_k^i in the sense that the difference $U_k^i - T(0)$ was approximately equal to the right side of (15) with the minus sign. Then $T(0) = (T_k^i + U_k^i)/2$ and

$$\left| T(0) - T_i^k \right| < \left| U_i^k - T_i^k \right|. \tag{16}$$

Such a bound U_k^i may be found, for example, as a linear combination $U_k^i = \sum_{j=0}^r \alpha_j T_k^{i+1-j}$ for appropriate values of indices. For $r = 1$, $\alpha_0 = 2h_i/(h_i - h_{i+k+1})$, $\alpha_1 = 1 - \alpha_0$ this is exactly the Bulirsch and Stoer bound canceling out $e_{k+1,0}$, the principal term on the right side in (15). The bound (16) provides a practical error estimate and thereby partially offsets the absence of any theoretical estimate.

The same techniques can be used in the case of polynomial extrapolation (then the coefficients (12) are not needed) since (15) and (13) have the same structure with respect to $h_1, \ldots, h_n$ and differ only by coefficients. Despite this equivalence, in practice, the rational extrapolation usually leads to better results both in the sense of accuracy and stability. For example, when $k_i = i$, $1 \le i \le n$, (Stehfest) the polynomial extrapolation, as already mentioned above, fails for $n = 16$ with using double precision arithmetic whereas the rational extrapolation works successfully. The comparison of accuracy given in Table 4 demonstrates the typical relationship.

4. INVERSION PROBLEM ON AN INTERVAL

Such inversion methods as the Fourier-series or Laguerre-series method enable one to solve the inversion problem on intervals $[0, T]$. The Post-Widder method also is applicable for this

Table 3. Application of the equalization procedure to the inversion of implicit function $\pi(s)$ determined from (21) $\beta(s) = 2/(2+s)$, $\lambda = 1$, $T = 4$; $k_j = 2^{j-1}$, $j = 1,\dots,8$, polynomial extrapolation at points $t_i = iT/256$. Error before and after equalization.

i	Error Before Relative	Error After Equalization Relative	Error After Equalization Absolute	i	Error Before Relative	Error After Equalization Relative	Error After Equalization Absolute
1	−1e − 3	−8e − 5	−1e − 04	133	−2e − 2	3e − 7	2e − 08
2	−2e − 4	−4e − 5	−7e − 05	134	3e − 4	−1e − 6	−8e − 08
3	−4e − 3	−1e − 4	−2e − 04	...	...	...	...
4	−5e − 5	−5e − 5	−8e − 05	191	−1e − 2	6e − 7	2e − 08
...	...	...	...	192	1e − 9	1e − 9	6e − 11
63	−2e − 2	−5e − 6	−1e − 06	193	−1e − 2	6e − 7	2e − 08
64	−4e − 7	−4e − 7	−9e − 08	194	2e − 4	−5e − 8	−2e − 09
65	−2e − 2	−4e − 6	−1e − 06	...	...	...	...
66	3e − 4	2e − 6	4e − 07	252	−3e − 6	3e − 8	6e − 10
...	...	...	...	253	−1e − 2	3e − 7	6e − 09
130	3e − 4	−3e − 7	−2e − 08	254	2e − 4	−2e − 9	−3e − 11
131	−2e − 2	7e − 7	5e − 08	255	−1e − 2	3e − 7	6e − 09
132	−3e − 6	−7e − 7	−6e − 08	256	−5e − 9	−5e − 9	−1e − 10

Table 4. Mixture of two out-of-scale exponential distributions with Laplace transform $\hat{f}(s) = 0.5/(10^{12} + s) + 0.5/(10^{-12} + s)$. Relative (at the top) and absolute (at the bottom) errors ($k_i = 4i$).

Extrapolation	$t = 10e - 12$	$t = 1$	$t = 10e + 12$
Polynomial	4e − 12	4e − 12	1e − 11
	3e − 12	2e − 12	2e − 12
Rational	3e − 14	1e − 14	2e − 13
	2e − 14	3e − 15	4e − 14

purpose. As has already been mentioned above, method (CS) with the desirable quantity $f_k(T)$ automatically computes also $k-1$ approximants of lower orders

$$f_1\left(\frac{T}{k}\right), \dots, f_{k-1}\left(\frac{(k-1)T}{k}\right), \qquad f_k(T). \tag{17}$$

One can reasonably dispose of them in order to reconstruct the sought function on the whole interval $[0,T]$ and not only at the endpoint T. The expressions (5) and (6) imply that even approximants of low order j can provide an appropriated accuracy if jT/n is sufficiently small. At last, when additional approximants are computed to use an enhancement procedure at the endpoint T, additional approximants are also obtained for some of the points jT/n, $1 \le j \le n-1$, which allows to apply some enhancement procedure at those points too. For definiteness we shall consider the situation when extrapolation to the limit is accomplished following Romberg, although similar considerations might just as well be applicable to other extrapolating sequences.

For fixed T let L_k denote the set of points $L_k = \{jT/2^{k-1} : 1 \le j \le 2^{k-1}\}$, $k = 1,2,\dots$ (net). Using (CS) repeatedly n times when k in (17) runs over the sequence $\{2^{q-1} : 1 \le q \le n\}$, we assign approximants to points of the nets $L_1 \subset L_2 \subset \cdots \subset L_n$ (the maximal number of passes, n, will be regarded as fixed throughout this section). As a result, each point of L_{n+1-q} is assigned not less than q approximants and each point of $L_{n+1-q} \setminus L_{n-q}$—exactly q, $q = 1,\dots,n$. In particular, at odd points of the most finely-graded net, L_n, there is only one approximant and at point T belonging to all nets there are n ones. It is clear that this unevenness in the number of associated to each point approximants leads to unwelcome hesitations of accuracy.

We consider two ideas providing the equalization with minimal extra computational work, both can be realized in a multiplicity of modifications. Unfortunately, an accurate error analysis of the procedures which would result is not likely possible in the light of such formulas as (5), (6), and (15).

The idea proposed in [18] as applied to differential equations transforms in the context of the the inversion problem as follows. Let $F_{k_q}(\cdot)$ denote the Lagrange polynomial constructed by interpolating the sequence (17) with $k = k_q = 2^{q-1}$ at points of L_q, $q = 1, \dots, n$. In order to evaluate the function at any point $t \in (0, T]$, the polynomial or rational extrapolation is applied to the numbers $F_{k_1}(t), \dots, F_{k_n}(t)$ being interpreted as original approximants. For practical use it is advisable to apply this approach for subintervals (just as recommended in [18]) resorting for the interpolation not all points but only some nearest neighbors of the point where the function is to be evaluated. Note that this approach is not restricted exceptionally to the sequences of imbedded nets but remains applicable when meshes of the nets do not have an integer common divisor.

The purpose of other heuristic approach is to increase accuracy at points belonging to $L_{n+1-q} \setminus L_{n-q}$ for given $1 \le q < n$, that is, at points where there are exactly q approximants. To give a rough idea, we introduce an auxiliary net function $\phi_q(\cdot)$ on L_{n+1-q} as the ratio of the sought value, $f(t)$, to its estimate, $f_q^*(t)$, constructed by polynomial or rational extrapolation using q highest available approximants. Then one can write $f(t) = f_q^*(t)\phi_q(t)$, $t \in L_{n+1-q}$. If the function $\phi_q(t)$ was known this formula could give the sought value. Since $\phi_q(t)$ is not known this formula is used to obtain approximate values, $f_q^{**}(t)$, by substitution of some approximate values $\phi_q^*(t)$ for exact ones $\phi_q(t)$

$$f_q^{**}(t) = f_q^*(t)\phi_q^*(t).$$

Such a function $\phi_q^*(t)$ at points $t \in L_{n-q}$ can be constructed, e.g., as the ratio $f_p^*(t)/f_q^*(t)$, where p is the number of approximants computed at t (consequently $p > q$) and thus $f_p^*(t)$ is the best estimate for $f(t)$ available by extrapolating to the limit. Then $\phi_q^*(t)$ extends to $L_{n+1-q} \setminus L_{n-q}$ by means of linear (for definiteness) interpolation using points $(\underline{t}, \phi_i^*(\underline{t}))$, $(\bar{t}, \phi_i^*(\bar{t}))$, where $\underline{t}$, $\bar{t}$ are nearest to t points of the net L_{n-q} such that $\underline{t} < t < \bar{t}$. The reason for introducing the function ϕ is that it is more suitable for interpolation than f itself. From (5) and (13), it follows that for $t_p \in L_{n+1-q}$, $p = 1, \dots, 2^{n-q}$

$$\begin{aligned} \phi_q(t_p) &= 1 + (-1)^q p^{-q} 2^{-q(q-1)/2} B_q(t_p), \\ \phi_q^*(t_p) - \phi_q(t_p) &= (-1)^q p^{-(q+1)} 2^{-(q+1)q/2} B_{q+1}(t_p), \end{aligned} \tag{18}$$

where by $B_q(t_p)$ is denoted the corresponding series and the second line is written for the worst case when the estimate $\phi_q^*(t_p)$ is obtained with using $q+1$ approximants. The error of the linear interpolation at $t_p \in L_{n+1-q} \setminus L_{n-q}$ can be expressed as

$$f(t_p) - f_q^{**}(t_p) = f_q^*(t_p)\left(\phi_q(t_p) - \phi_q^*(t_p)\right) \approx (t_p - \underline{t}_p)(t_p - \bar{t}_p)\,\phi_q\left[\underline{t}_p; t_p; \bar{t}_p\right]. \tag{19}$$

The formulas (18) and (19) imply that $f(t_p) - f_q^{**}(t_p)$ is to be of higher order in $1/p$ than $f(t_p) - f_q^*(t_p)$ if $B_p[\underline{t}_p; t_p] = o(1)$ and $B_p[\underline{t}_p; t_p; \bar{t}_p] = o(p^{-1})$. Although there are grounds for believing that this is really so when dealing with sufficiently smooth and slowly varying functions, yet it does not seem possible to rigorously prove this fact, especially in the case of estimates $f_q^*(t_p)$ obtained by rational extrapolation. In practice this approach demonstrates good results (see Table 3) and is easy in implementation.

5. INVERTING MULTIDIMENSIONAL LAPLACE TRANSFORMS

Choudhury, Lucantoni and Whitt [23] considered the problem of inverting multidimensional Laplace transforms. Here, we briefly discuss how the results of previous sections can be easily extended to functions of several arguments. In the present discussion, we restrict ourselves to the case of two variables. From theoretical point of view there is no loss of generality in this restriction and from practical point of view computational problems in this case are quite surmountable.

By the same arguments as in the one-dimensional version it can be shown that the approximants are of the form

$$f_{k_1\,k_2}(t,x) = rs\frac{(-r)^{k_1-1}(-s)^{k_2-1}}{(k_1-1)!(k_2-1)!}\frac{\partial^{k_1+k_2-2}}{\partial r^{k_1-1}\partial s^{k_2-1}}\widehat{f}(r,s)\bigg|_{r=k_1/t,\, s=k_2/x},$$

and have the error estimate of the same structure as in (5),(7) which using reciprocals $h_1 = 1/k_1$, $h_2 = 1/k_2$ takes the form

$$T(h_1,h_2) = f_{k_1\,k_2}(t,x) = f(t,x) + \sum_{n\geq 1}\sum_{m=0}^{n} a_{m\,n-m}(t,x)h_1^m h_2^{n-m}, \tag{20}$$

where the coefficients $a_{n_1n_2}(t,x)$ are independent of k_1 and k_2 when the function f is infinitely differentiable.

Again values of approximants can be obtained by any of the methods mentioned in Section 2. In particular, methods (TI) and (CS) are based on the following formula

$$rs\widehat{f}(r(1-z), s(1-u)) = \sum_{n_1,\,n_2\geq 1} f_{n_1n_2}\left(\frac{n_1}{r}, \frac{n_2}{s}\right) z^{n_1-1}u^{n_2-1}$$

directly generalizing (2). Program implementation of method (CS) is based on a set of subroutines performing operations on two-dimensional series, which reduce to the operations on one-dimensional series.

For example, let the Laplace transform $\widehat{F}(r,s)$ be represented as a ratio of two functions. Thus, $\widehat{F}((1-z)r,(1-u)s) =: C(z,u) = A(z,u)/B(z,u)$ for some functions A and B. One can write

$$A(r(1-z), s(1-u)) = \sum_{i\geq 0} a_i(z)u^i, \quad B(r(1-z), s(1-u)) = \sum_{i\geq 0} b_i(z)u^i,$$

where $a_i(\cdot)$, $b_i(\cdot)$, $i \geq 0$ are one-dimensional series. Then series $c_i(\cdot)$ in the analogous expansion for C are obtained from (4), where, however, arithmetic operations should be treated as operations on the series. Thus, $f_{k_1,k_2}(t,x) = c_{k_1,k_2}/(s_0r_0)$ with $r_0 = k_1/t$, $s_0 = k_2/x$.

As follows from (20) the extrapolation to the limit on $h_1 = 1/k_1$ and $h_2 = 1/k_2$ is possible. Since the number of coefficients of the interpolating function must be equal to the number of interpolating points, it seems to be reasonable to recast the two-dimensional problem in one-dimensional by putting $k_1 = \alpha k_2$ for some rational α in which case, as follows from (20), the number of unknowns can be significantly reduced. Then, all considerations presented in foregoing sections remain in force. In particular, the same procedures of polynomial and rational extrapolation can be used without any changes.

6. NUMERICAL EXAMPLES

The efficiency of the procedures described in the paper is illustrated by Tables 2–4. Since values of the inverted transforms in themselves are not interesting in the context of the present discussion, the tables contain only deviations between inverted and true values. It should be noted (one more time) that all these results were obtained using standard double precision arithmetic. In all of the examples original approximants were calculated with method (CS). In Table 2, $J_0(t)$ is the Bessel function, $\widehat{J_0}(s) = 1/\sqrt{s^2+1}$, the function $M(t)$ was discussed by Jagerman [3]. Inverting an implicit function is demonstrated for the function $p(t)$ with Laplace transform $\pi(s)$ defined as the solution to the equation

$$\pi(s) = \beta(s + \lambda - \lambda\pi(s)), \tag{21}$$

where $\beta(s)$ is the known Laplace transform of a probability density function and λ is a nonnegative number. Remark that the data for $\pi(\cdot)$ in Tables 2 and 3 were obtained with the computational procedure [11] which did not rely on the exponential form of $b(\cdot)$. The example of a mixture of two exponential out-of-scale distributions (Table 4) was discussed by Abate and Whitt [7]. Table 4 also illustrates the superiority of rational extrapolation to the limit over polynomial, the choice of interpolating sequence being the same. The results contained in Table 3 was obtained in two steps. First, the values was corrected at points of L_{n-3} and then, on the basis of these corrected values,—at all remaining points.

The two-dimensional version of the method is illustrated with the inversion of the function (the Beneš formula)

$$\widehat{W}(r,s) = r\frac{u(r) - u(s+\lambda-\lambda\pi(s))}{s - r + \lambda - \lambda\beta(r)}$$

whose original in queueing theory is interpreted as the time dependent distribution of the virtual waiting time and in the risk theory as the distribution of the current capital [24]. Here $u(r) = \omega(r)/r$, $\omega(r)$, and $\beta(r)$ are known Laplace-Stieltjes transforms of the initial waiting time and service time distributions, respectively, $\pi(s)$ is determined from (21).

In realization, approximants were computed with method (CS). The function was evaluated in rectangle areas with the Romberg nets. For the maximal order of approximant 32 for each argument the relative error achieved (after equalization) typically 10^{-5}–10^{-7} as at the best points (with the number of approximants 3–5).

7. CONCLUSION

By combining one of the above techniques for calculating original approximants and one of the variants of extrapolation to the limit one can construct different members of the family of Post-Widder inversion methods. For example, the representatives previously discussed in the literature are following: (FD) + Romberg [4], (FD) + Stehfest [6], (TI) + Stehfest [7] (in all these cases polynomial extrapolation was used). Our experience allows to conclude that by using (CS) and rational extrapolation instead of polynomial a better accuracy can be achieved as applied to the inversion of implicit functions.

The Post-Widder method turns out to be sufficiently universal and convenient because it has no free parameters to be tuned and admits implementations both those using only values of $\widehat{f}(\cdot)$ (with (TI)) and those using coefficients of its Taylor expansion (2) (with (CS)). In accuracy and time it is competitive with other methods acknowledged to be the most accurate, e.g., the Laguerre-series method in Piessens and Branders' version [8] and variants of the Fourier-series method including that due to Honig and Hirdes [25] with double error correction. A comparison with discussion is given in [11].

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